Development of High-Performance and High-Accuracy Computational Fluid Dynamics Method for Interfaces

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To understand fluid dynamics, including multiphase flows, the equation with moving boundaries comprising the interfaces must be solved. This study introduces the volume of fluids (VOF) and level set (LS) methods. Consequently, the coupling techniques between the VOF and LS methods, and our proposed method are reviewed. The proposed method can reduce computational load and exhibits high accuracy. Finally, we demonstrate that the proposed method can visualize and contribute to the understanding of various flow phenomena.

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Introduction

Problems involving fluids cannot be avoided when dealing with industrial processes. Kajishima[1] defined fluid as "a concept that deals mechanically with substances represented by gases and liquids." The laws of conservation of mass, momentum, and energy (and equations of state) are discussed under this definition. In particular, the law of conservation of momentum is called the Navier-Stokes equation, and fluid mechanics researchers have struggled with this equation since the 19th century, when it was established, to the present day. After the emergence of electronic computers in the 1950s, many researchers have debated on ways to solve the Navier-Stokes equation and established this issue as a third field of research alongside experiment and theory. The struggles in these endeavors are described in the pioneering book "Computational Fluid Dynamics" (1978)[2].

The initial fluid simulations involved computations for the flow of a single component of gas or liquid. To solve the Navier-Stokes equation, which is a partial differential equation, specific boundary conditions, such as walls and inlets, *etc.*, must be established. These boundary conditions had to be spatially fixed, or it would have been difficult to solve the equation with the available performance of computers at the time. Meanwhile, fluids in which multiple phases are mixed, such as gas and liquid, or two immiscible liquids (water and oil), are found in many industrial devices. **Fig. 1** shows representative examples. These are called two-phase or multiphase flows. In these cases, the Navier-Stokes equation holds for the liquid side or the gas side, but the interface that separates the liquid and gas moves freely in space. In other words, the position where the boundary condition is imposed can move freely, which leads to an even more difficult computational field, referred to as the moving boundary problem.

Research is ongoing on the moving boundary problem in the fields of physics, mathematics, and engineering, but developments are also expected in the fields of physiology, medicine, and chemistry in the future. As indicated by Dr. Nurse[3] and many other researchers, the boundary (*e.g.*, cell walls of living organisms) controls entropy and constitutes an evolving phenomenon that successfully resists the chaotic forces that permeate the entire universe. Additionally, the moving boundary problem should be discussed for the self-organization of functional materials.

In terms of simulations, until the 1980s, emphasis

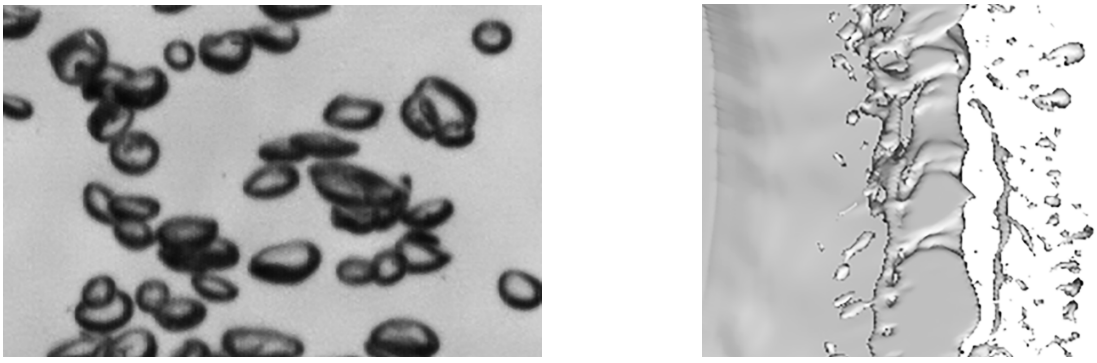


Fig. 1 Examples of flows with two immiscible fluids (left: experimental snapshot of a rising bubble swarm in liquid, right: simulated atomization at the leading edge of a rotating liquid film)

was placed on industrial practicality, with a focus on modeling the interphase velocity difference. These models have evolved into homogeneous flow models, slip flow models, drift flux models, and two-fluid models[4]. Modeling of the interphase velocity difference is complemented with idealized analytical solutions or experimental data. In other words, the accuracy of the computations largely depends on this modeling. If the modeling assumptions are correct, then there are no problems. However, not all interfaces that actually exist necessarily satisfy the assumptions. For example, it is difficult to solve for a freely deformable interface (**Fig. 1**).

In the 1990s, several computational methods were proposed for solving the deforming interface directly with the objective of overcoming the above-mentioned problems. Examples include the volume-of-fluid (VOF) method, level set (LS) method, front-tracking method[5], boundary fitting coordinate method[6], lattice Boltzmann method, and phase field method. In this paper, we provide an overview of the VOF method and the LS method, which are often used in many simulation codes. Next, we explain the coupling method of the new VOF method and LS method developed by the authors in recent years, and application examples.

Interface capturing method

Both the VOF and LS methods are used for discriminating between the phases of fluids, and the underlying basic concepts are mostly similar. However, the problems of numerical computation and the history of its improvements differ. To simplify the explanation, we consider a two-phase flow in which the gas and liquid are in the computational domain. In the VOF method, we identify a volume fraction α. For example, if $\alpha = 1$, then it is a gas, and if $\alpha = 0$, then it is a liquid. If $0 < \alpha < 1$, then both gas and liquid are contained, which signifies that an interface exists. Meanwhile, in the LS method, a signed distance function ϕ from the interface is used. If $\phi = 0$, then it is an interface, if $\phi > 0$, then it is a gas, and if $\phi < 0$, then it is a liquid. The technical problem is in the computation of α or ϕ moving in space.

1. VOF method

First, when calculating the spatial movement of α, we must first eliminate diffusion, which cannot physically occur, and any computations for which $\alpha > 1$ or $\alpha < 0$. Hirt[7], who was a pioneer of the VOF method, introduced the donor-acceptor method. The multi-interface advection and reconstruction solver (MARS) method[8], piecewise linear interface calculation (PLIC) method[9], high resolution interface capturing (HRIC) method[10], and compressive interface capturing scheme for arbitrary mesh (CICSAM) method[11] were proposed as further improvements of the donor-acceptor method.

The accuracy is certainly improved by these methods, but there is a high computational load imposed by them. In 2005, Xiao[12] proposed a simpler and more accurate method of moving α by using the hyperbolic tangent function. This method is called the tangent of hyperbola for interface capturing (THINC) method. Next, in 2007, Yokoi[13] proposed a computational method that combines the weighted line interface calculation (WLIC) method and the THINC method. This improved the accuracy of multi-dimensional computations. These methods do not require iterative computations, which led to faster computations. Furthermore, in 2013, we developed a method that adjusts the hyperbolic tangent function using an adaptive slope[14], whereby

they improved the accuracy in multiple dimensions while maintaining simplicity and fast computational speeds. Therefore, the developed method is called the tangent of hyperbola with adaptive slope for interface capturing (THAINC) method.

2. LS method

While α can have a sharp distribution between 0 and 1, ϕ represents a signed distance from the interface; therefore, it has a continuous distribution. We calculated the spatial derivative $\nabla\phi$. The error is negligible especially when computing the surface tension, as the spatial derivative needs to be taken to calculate the interface and curvature. Sussman *et al.*[15] first applied the LS method to a gas-liquid two-phase flow in 1994.

An important technique in this method is the re-initialization operation of ϕ. When spatially moving ϕ, the properties of ϕ as a signed distance function may be lost as a result of accumulated numerical errors. Therefore, a re-initialization operation is conducted to restore the property as a signed distance function. It has been indicated that the volume conservation properties of the target fluid are lost during the re-initialization operation. Hartmann *et al.*[16] proposed an improved re-initialization method to overcome this issue. We[17] have also previously proposed a re-initialization method that does not produce errors even when the position of ϕ = 0 changes, to consider stacking and phase change phenomena.

3. Combination of VOF method and LS method

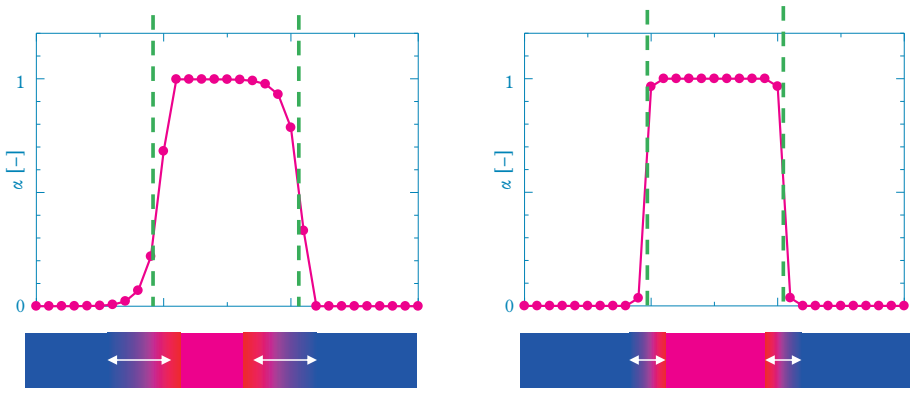
In the 2000s, when the VOF and LS methods were developed and their strengths and weaknesses became known, a combination of these methods emerged. This combination allowed for each method to complement each other's weaknesses. For example, the VOF method is used to track the fluid of interest, and the LS method is used to compute the curvature and normal vector. This is termed as the coupled LS and VOF (CLSVOF)[17] method. The CLSVOF method is still widely recognized today as a method with a higher computational accuracy than other methods. However, its computational load is high. Not only do α and ϕ both need to be computed, re-initialization of ϕ also becomes necessary. Therefore, in 2013, Albadawi *et al.*[18] attempted to combine the VOF method and LS method in a simpler way. This is a simple version of the CLSVOF method; therefore, it is commonly referred to as the simple coupling LS and VOF (S-CLSVOF) method.

In the S-CLSVOF method, ϕ is built from α based on algebraic expressions, but it is difficult to say that the advantages of ϕ are fully utilized, given that the spatial distribution information is not considered. Therefore, we propose a computational method for obtaining ϕ from α by utilizing the previously-mentioned THAINC method. This method allows for the spatial distribution information to be reflected in ϕ with an adaptive slope. Furthermore, the computational load hardly increases, and the simplicity is not lost. In this report, this improvement is termed as the improved S-CLSVOF method[19].

4. Demonstration of developed method

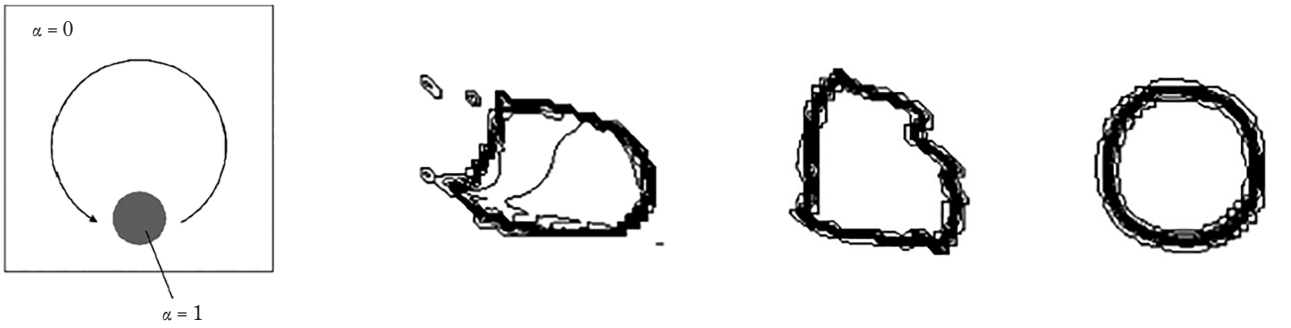
(1) Accuracy of spatial movement by THAINC method

Fig. 2 shows a test example in which α is moved one-dimensionally from left to right. The HRIC method, which is often used in commercial software, is shown under the same computational conditions for comparison. For example, α is used to discriminate the phase



(a) HRIC method (b) THAINC method

Fig. 2 Numerical test of one-dimensional advection of α (from the left to right)



(a) Test condition (b) Donor-Acceptor method (c) THINC method (d) THAINC method

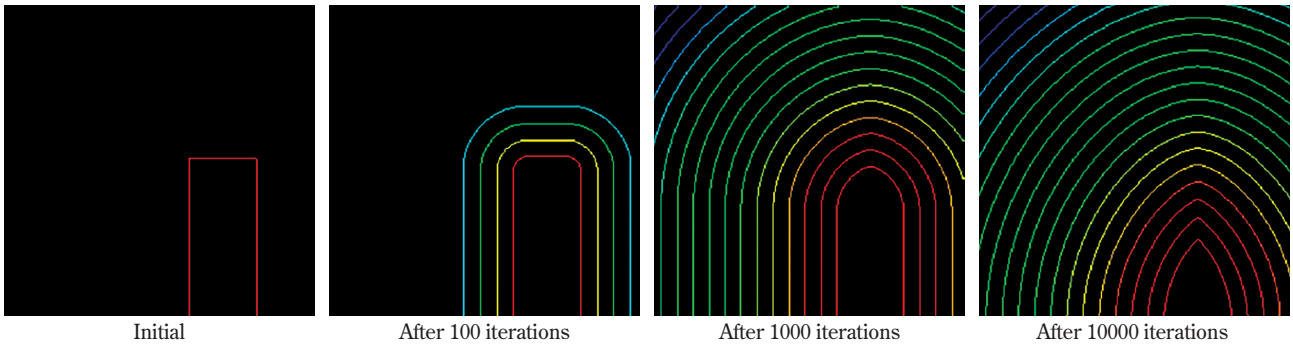
Fig. 3 Numerical test of two-dimensional rotational advection of α[14)]
(the line indicates the contour of $0 \leq \alpha \leq 1$)

such that $\alpha = 0$ for liquids and $\alpha = 1$ for gas. In the HRIC method, the $0 < \alpha < 1$ domain is slightly expanded. This can be a non-physical error factor of interface diffusion. Meanwhile, in the THAINC method, the $0 < \alpha < 1$ domain is narrow, and it can be seen that this is more effective for phase discrimination.

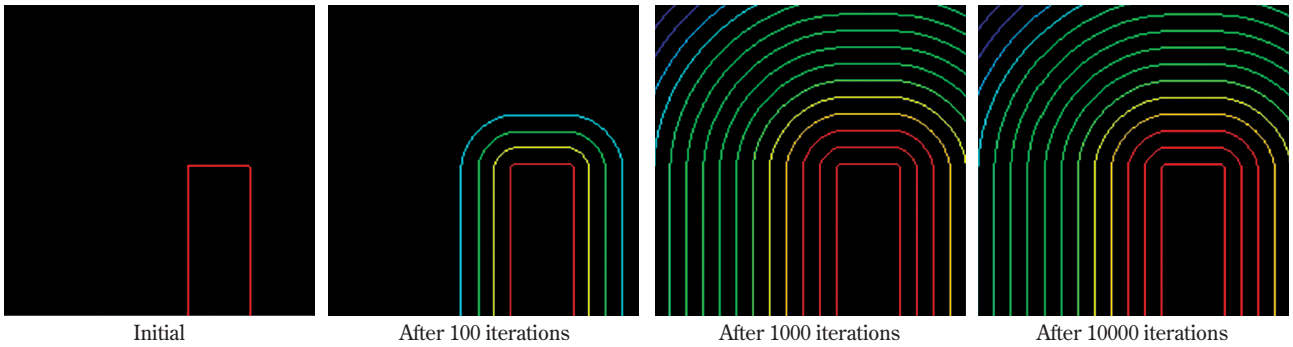
Fig. 3 shows the results of two-dimensional testing. If the circle is rigidly rotated on a plane and retains the same shape and area as previously, then it signifies that the accuracy is that much higher. The circle shape was well preserved in the THAINC method, whereas the circles were greatly distorted in the donor-acceptor method and THINC method, which were used for comparison. The area conservation was on the order of 10^{-11}, which was about the same as the truncation error of double-precision computations on computers.

(2) Re-initialization of LS method

Fig. 4 shows a comparison of ϕ re-initialization methods. We first place a rectangle, as indicated by the red



(a) Original re-initialization method



(b) Proposed re-initialization method

Fig. 4 Comparison between two-dimensional re-initialization methods for ϕ[17)]

lines, and when we conduct the re-initialization computation, lines are drawn outside the rectangle so that ϕ is the distance from the red lines. Based on the definition of ϕ, the lines are composed in equal intervals, but in the original re-initialization method, the shape of the red rectangle created at the beginning collapsed, and the area became smaller. This was the problem with the early LS method. As previously mentioned, it can be seen that the re-initialization method proposed by the authors maintains the shape and area of the red rectangle.

(3) Surface tension accuracy by improved S-CLSVOF method

Fig. 5 shows the surface tension test of two-dimensional bubbles. If bubbles are arranged in a circle in a liquid in zero-gravity space, then the pressure caused by the surface tension (Laplace pressure) balances the pressure field of the surrounding fluid, and the bubble remains circular and stationary. In the VOF method, as shown in **Fig. 5**(a), it is known that computational errors in the surface tension result in the loss of pressure balance, generating a flow near the interface and causing the bubbles to vibrate without maintaining a circular shape. This is a problem referred to as parasitic current, and many technical developments have been proposed for overcoming this problem. As shown in **Fig. 5**(b), the parasitic current can be considerably suppressed in the original S-CLSVOF method by Albadawi *et al.*[18]. This also shows that the introduction of the LS function ϕ is effective in the computation of surface tension. Additionally, the improved S-CLSVOF method proposed by the authors can further reduce the parasitic current, as shown in **Fig. 5**(c).

(4) Examples of various two-phase flow computations

Finally, we demonstrate how the computational methods explained above can help visualize various fluid phenomena and contribute to our understanding of them. **Fig. 6** shows bubbles generated from a nozzle. The figure is axisymmetric in two dimensions, and the left end of the black line indicates the axis of symmetry. It can be seen that the flow path of the gas narrows, and the flow accelerates just before the bubble leaves the nozzle. We confirmed that there was no difference in the bubble behavior even when compared with the CLSVOF method, which has a high accuracy and a high computational load.

Fig. 7 shows that, as the bubble rises, a black-colored liquid is lifted upwards. It is difficult to predict such a phenomenon unless the interface is accurately captured and the fluid is computed.

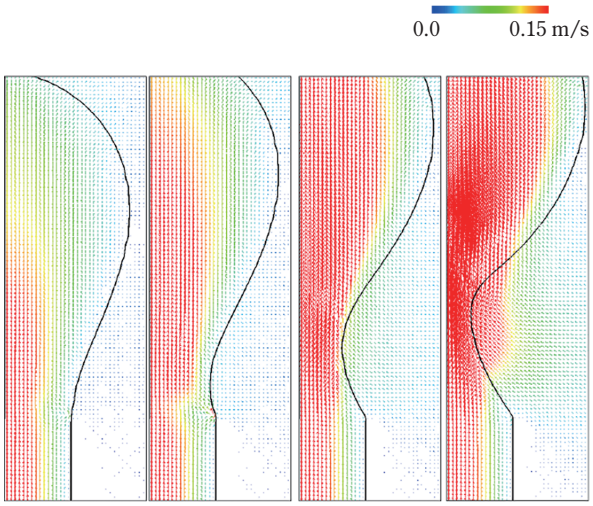
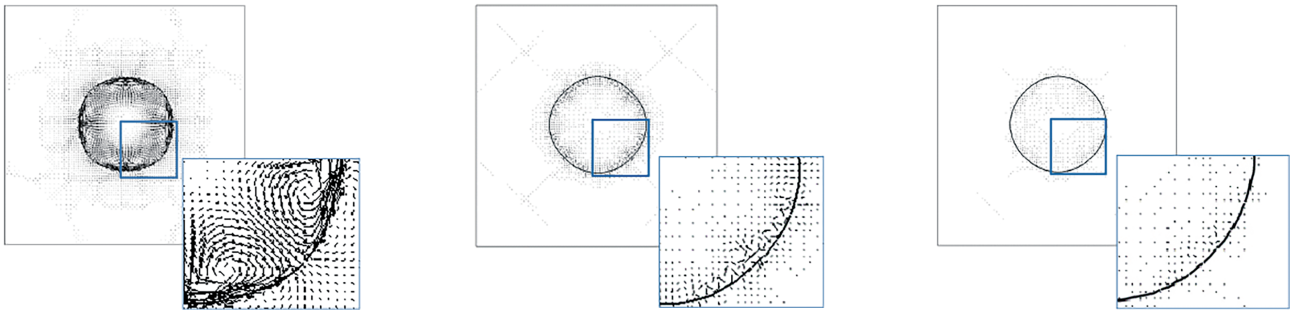


Fig. 6 Simulation of a bubble generated from a nozzle



(a) VOF method (b) Original S–CLSVOF (c) Modified S–CLSVOF

Fig. 5 Surface tension test on a two-dimensional bubble

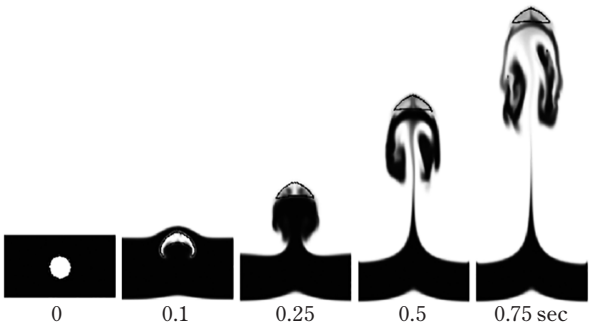


Fig. 7 Simulation of liquid entrainment via a single bubble[14)]

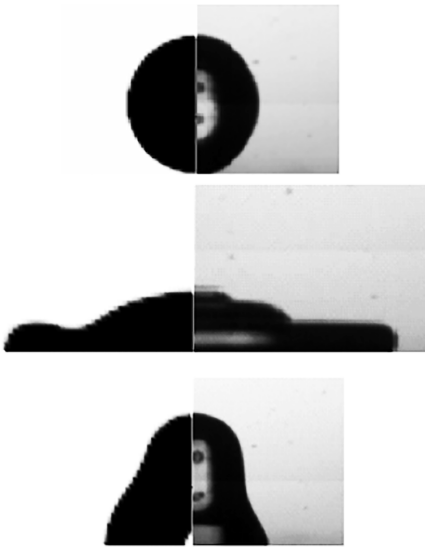


Fig. 8 Droplet wetting on a plate[14)] (from the top: 0, 2, 10 ms)

Fig. 8 shows how the droplet collides with a solid wall. The right half of the figure is the observation result from a high-speed camera, and the left half is the simulation result. It can be seen that the behavior of a nearly spherical falling droplet colliding with the wall surface, flattening in the horizontal direction, and then trying to rebound upward again is well reproduced. **Fig. 9** compares how a droplet slides down an inclined plate. **Fig. 9**(a) is the result of an observation with a high-speed camera. The droplet moves from the upper left to the lower right in the figure, but the angle at which the droplet comes into contact with the plate at the lower right (advancing angle) and the angle at which the droplet comes into contact with the plate at the upper left (receding angle) are different. These angle problems have been well reported experimentally, and they sometimes become important in functional materials as well. However, they have not been completely clarified on a theoretical level. For example, Young's equation is often described in the literature as surface wettability, *etc*., but the discussion is limited to a balance of forces in the tangential direction, with no explanation on the normal direction and friction. It should also be noted that many types of software do not automatically compute the dynamic contact angle, but instead require the input of empirical values. As shown in **Fig. 9**(b), when statically measuring the contact angle, the advancing angle and receding angle are not distinguished, which results in a different shape from that of an actual droplet. We are working on revising **Fig. 9**(c) by combining the equation by Jiang *et al*.[20)]

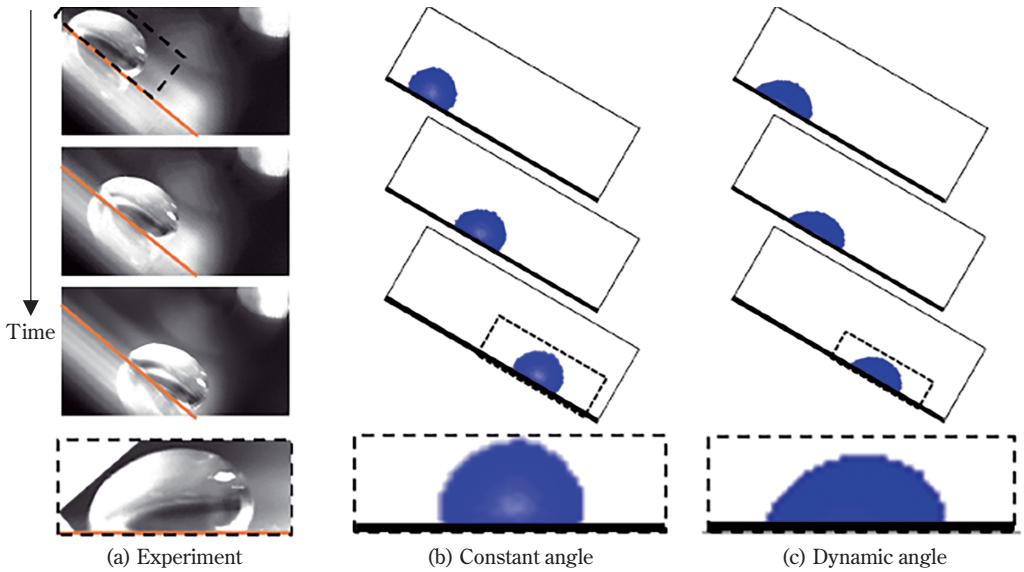
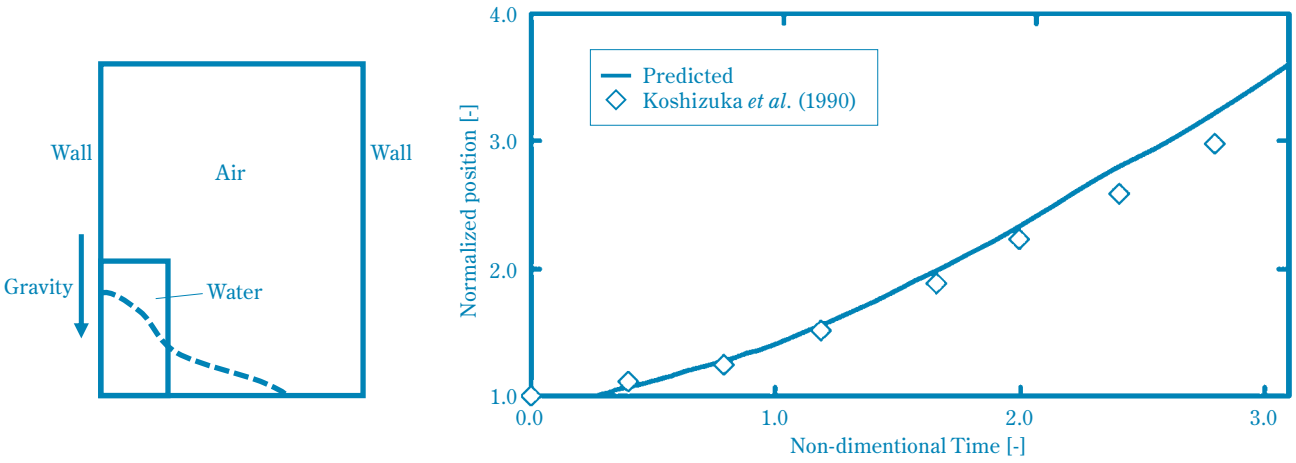


Fig. 9 Simulation of a single droplet slipping on an inclined plane

for the advancing angle and the Hoffman-Voinov-Tanner equation[21] for the receding angle as a prescriptive method that considers practicality. Although this comes close to the trends seen in experiments, it still cannot be called a universal model. Albeit this seems like a simple phenomenon at first glance, it is a very difficult problem in which microscale conditions need to be connected to macroscale phenomena, such as the roughness and nonuniformity of solid surfaces, friction between gas and liquid, and changes in surface tension.

Fig. 10 indicates the problem of a liquid column collapse. Initially, the liquid is placed in a rectangular shape in the lower left corner of the domain. Over time, the liquid begins to collapse owing to gravity, moves to the right at the bottom, and eventually collides with the right wall. This problem is often discussed in terms of a dam collapse or tsunami problem. **Fig. 10**(b) shows a graph comparing the computed liquid tip velocity with the experimental results by Koshizuka *et al.*[22]. This method shows good agreement with the experimental results.

Fig. 11 is a computational example of spin coating. For the purpose of computational efficiency, this was made axisymmetric in two dimensions, with the dashed line in the left being axially symmetrical. The red part of the figure represents the liquid, and the blue part represents the gas. The liquid spread outward (to the right in the figure) owing to the centrifugal force, and during this process, the film thickness of the liquid changed by several dozens of micrometers.



(a) Numerical condition

(b) Comparison of tip velocity

Fig. 10 Predicted collapse of a liquid column

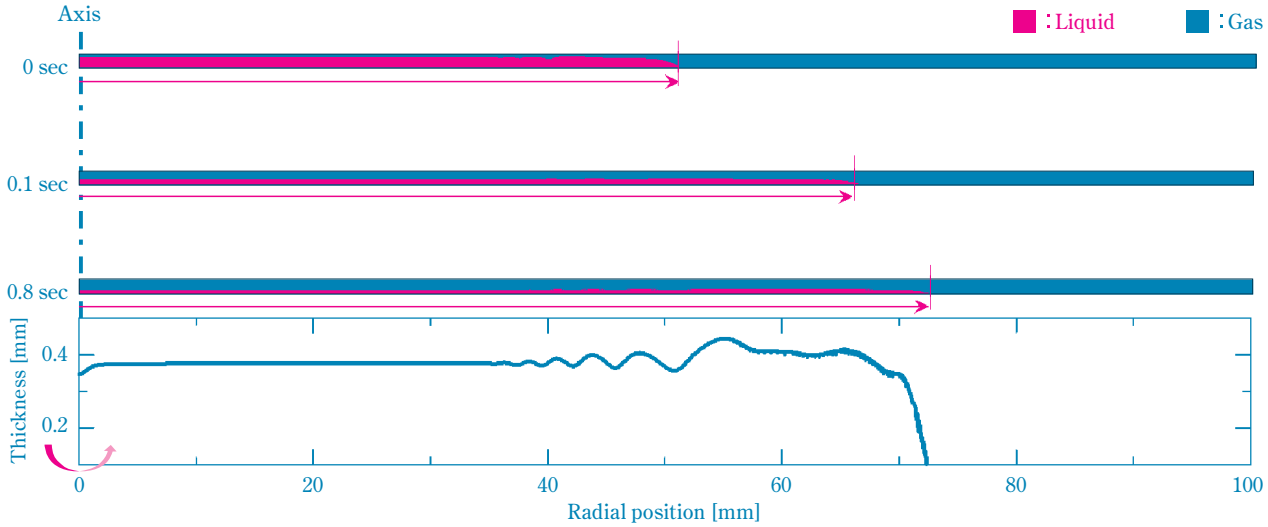


Fig. 11 Simulation of a spin coating

Conclusion

We introduced a simulation technique to compute the two-phase interface in the form of a moving boundary problem. As a separate problem, simulations of interactions between solids and fluids are being extensively studied. This is also called fluid structure interaction (FSI). In a previous paper, we introduced a high-speed computational method based on the cut-cell method[23], which can also be seen as a form of FSI. However, it is empirically known that the convergence of the computation decreases when the solid is moved in space. Therefore, the authors are also developing other methods, such as the immersed boundary method (IBM). These findings indicate that simulations are still not a perfected technology (*i.e.*, computers do not do them automatically) and that they need to be continuously developed based on deep insights into various phenomena. Furthermore, hardware performance is expected to improve dramatically in the future; therefore, ways to leverage these benefits should always be a point of consideration. We hope that this paper will be of at least some help to the readers.

Reference

1) T. Kajishima, Ryutaikogaku no Kiso [Introduction of Fluid Dynamics], Morikita Shuppan, (2002).
2) P. J. Roche, Computational Fluid Dynamics, Hermosa Publishers (1978).
3) P. Nurse, What is Life? – Understand Biology in Five Steps, David Fickling Books (2020).
4) Atomic Energy Society of Japan, Thermal Hydraulics Division, Ed., Kiekinisoryu no Suchikaiseki [Numerical Analysis of Two-phase Flows], Asakura Shoten (1993).
5) M. Ohta *et al.*, Konsoryu no Suchishimyureshon [Numerical Simulation of Multiphase Flows], Maruzen Shuppan (2015).
6) S. Koshizuka, Suchiryutairikigaku [Computational Fluid Dynamics], Baifukan (1997).
7) Hirt, C. W. and B. D. Nichols, J. Comput. Phys., 39, 209 (1981).
8) T. Kunugi, Trans. JSME Ser. B, 63, 1576 (1997).
9) W. J. Rider and D. B. Kothe, J. Comput. Phys., 141, 112 (1998).
10) T. Waclawczyk and T. Koronowicz, J. Theor. Appl. Mech., 46, 2, 325 (2008).
11) O. Ubbink and R. I. Issa, J. Comput. Phys., 153, 26 (1999).
12) F. Xiao, *et al.*, Int. J. Numer. Meth. Fluids, 48, 1023 (2005).
13) K. Yokoi, J. Comput. Phys., 226, 1985 (2007).
14) A. Dhar *et al.*, Kagaku Kougaku Ronbunshu, 39, 2, 86 (2013).
15) M. Sussman *et al.*, J. Comput. Phys., 114, 146 (1994).
16) D. Hartmann *et al.*, J. Comput. Phys., 229, 1514 (2010).
17) K. Sodeyama *et al.*, Kagaku Kougaku Ronbunshu, 46, 3, 49 (2020).
18) A. Albadawi *et al.*, Int. J. Multiphase Flow, 53, 11 (2013).
19) N. Shimada *et al.*, 4th Int. Symp. Multiscale Multiphase Process Eng. (2022).
20) T. S. Jiang *et al.*, J. Colloid and Interface Sci., 69, 1, 74 (1979).
21) R. Hof fmann, J. Colloid and Inter face Sci., 50, 2, 228 (1975).
22) S. Koshizuka and Y. Oka, Nucl. Sci. Eng. 123, 421
23) N. Shimada, SUMITOMO KAGAKU, 39 (2021).

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